The Entropy Density of Quasi-Free States

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ABSTRACT: The problem of deriving an explicit expression for the entropy density of an Euclidean and gauge invariant quasi-free state of the CCR algebra is discussed. An expression is conjectured and it is shown that this provides a lower bound for the entropy density. In the course of this a general theorem on the trace of a function of the Laplacian is proved.

RÉSUMÉ: On discute le problème de dériver une expression explicite pour la densité d'entropie d'un état quasi-libre invariant des groupes euclidiens et jauge de l'algèbre de relations de commutation. On propose une expression et on montre que celle-ci est un minorant de la densité d'entropie. Au cours de cette démonstration on prouve un théorème générale sur la trace d'une fonction du laplacien.

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1. STATEMENT OF RESULTS

In this note we discuss the problem of obtaining an explicit formula for the entropy density of an Euclidean-invariant, gauge-invariant quasi-free state of a boson system analogous to that given by Fannes [10] for Fermi lattice systems. We conjecture that formula (1.3) below provides this realisation, but we have succeeded in proving only that it is a lower bound for the entropy density.

Let $\mathfrak{A}$ be the algebra of the canonical commutation relations (CCR) over the test function space $C_c^\infty(\mathbb{R}^3)$ of infinitely differentiable functions of compact support. $\mathfrak{A}$ can be identified with the norm closure of the union of local Weyl algebras:

$$\mathfrak{A} = \overline{\bigcup_{|\Lambda|<\infty} \mathfrak{A}(\Lambda)}$$

The states of $\mathfrak{A}$ that are of physical interest are the locally normal states since, as observed by Dell'Antonio, Doplicher and Ruelle [9], they correspond to systems in which a finite volume contains a finite number of particles. A locally normal state is determined by a sequence of compatible density matrices $\{\rho_\Lambda\}$ ('compatible' as used by Robinson [16] p. 94), where ρ_Λ determines a state on the local algebra $\mathfrak{A}(\Lambda)$. Araki and Lieb [2] proved the existence of the entropy density $s(\omega)$ of a translation invariant locally normal state ω, defining it as the limit of the local entropy densities:

$$s(\omega) = \lim_{|\Lambda|\to\infty} -|\Lambda|^{-1}\,\mathrm{trace}(\rho_\Lambda \log \rho_\Lambda) \quad , \tag{1.1}$$

this limit being taken through a sequence of cubes, or more general regions made up of cubes. Robinson [16] (pp. 100-104) showed that as a function on the set of periodic states of $\mathfrak{A}$, the entropy density so defined is upper semi-continuous in the weak*-topology. Thus if $\{\omega_n\}$ is a sequence of periodic states converging to ω in the weak*-topology then

$$\limsup s(\omega_n) \leqslant s(\omega) \ . \tag{1.2}$$

A gauge invariant quasi-free state ω on $\mathfrak{A}$ is determined by a positive operator B defined on $C_c^\infty(\mathbb{R}^3)$ (see § 2). We assume that ω is Euclidean invariant so that B is a function of the Laplacian: $B = b(-\Delta)$. We conjecture that the entropy density of ω can be expressed in terms of the function b in the following way:

$$S(\omega) = \int_{\mathbb{R}^3} \{ (1 + b(|k|^2)) \log(1 + b(|k|^2)) - b(|k|^2) \log b(|k|^2) \} \frac{d^3k}{(2\pi)^3} . \qquad (1.3)$$

Our justification for this rests on the following argument. Under certain conditions on the function b we show (Theorem 2) that ω can be approximated by a sequence of normal states $\{\omega_L\}$, each given in terms of the Laplacian Δ_L on a bounded region Λ_L. (The restrictions to be placed on the sequence $\{\Lambda_L\}$, and the boundary conditions imposed on the local Laplacians Δ_L are discussed in sections 2, 3 and 4.) The entropy of a normal quasi-free state can be expressed as the trace of a function of the operator B (theorem 3); in our case this reduces to the trace of a function of the local Laplacian Δ_L. So to investigate the behaviour of the sequence $\{ |\Lambda_L|^{-1} S(\omega_L) \}$ of entropy densities we prove (in section 3) the following trace formula for functions of the Laplacian:

THEOREM 1: Let $f : \mathbb{R}^+ \to \mathbb{R}$ be a bounded, differentiable function such that $f' \in L^1_{loc}(\mathbb{R}^+)$ and which is eventually decreasing. Then the following conditions are equivalent:

(i) trace $f(-\Delta_\Lambda)$ exists for some region Λ.

(ii) $\int f(|k|^2)\, d^3k$ exists.

(iii) trace $f(-\Delta_L)$ exists for each L.

Furthermore, if one of the above holds then

$$\lim_{L\to\infty} |\Lambda_L|^{-1} \operatorname{trace} f(-\Delta_L) = \int_{\mathbb{R}^3} f(|k|^2) \frac{d^3k}{(2\pi)^3} .$$

[Δ_Λ, occurring in (i), is the Laplacian on the open region Λ together with a suitable boundary condition (see sections 2 and 3). Λ is not necessarily a member of the sequence $\{\Lambda_L\}$. This theorem, which was suggested by a lemma of Davies [8], is of independent interest, so it is stated and proved in greater generality in section 3 (theorem 5). In section 2 we use it to show that $\lim_{L\to\infty} |\Lambda_L|^{-1} S(\omega_L)$ is equal to the right hand side of (1.3).

In section 4 we prove that $\{\omega_L\}$ converges to ω in the weak*-topology. Thus from (1.2) we have proved that

$$S(\omega) \geq \int_{\mathbb{R}^3} \{ (1 + b(|k|^2)) \log(1 + b(|k|^2)) - b(|k|^2) \log b(|k|^2) \} \frac{d^3k}{(2\pi)^3} . \qquad (1.4)$$

In section 5 we show that the conditions we impose on b in order to prove the theorems are satisfied by a non-trivial class of functions. In particular they are satisfied in the case of the free boson gas above the transition temperature. Verbeure [22] has informed us that there is unpublished work on this subject by himself and by Lanford and Robinson.

§ 2. ENTROPY DENSITY

Let W be the Fock representation of the CCR over $C_c^\infty(\mathbb{R}^3)$ (as described, for example, by Cannon [4]). Since $\mathcal{O}\!\mathcal{l}$ is generated by the set $\{W(h) : h \in C_c^\infty(\mathbb{R}^3)\}$ it follows that a state ω on $\mathcal{O}\!\mathcal{l}$ is completely determined by the generating functional $\mu : C_c^\infty(\mathbb{R}^3) \to \mathbb{C}$ defined by

$$\mu(h) = \omega(W(h)) .$$

A state is gauge invariant if its generating functional is invariant under the transformation $h \mapsto e^{i\theta} h$; it is Euclidean invariant if its generating functional is invariant under the obvious induced action on $C_c^\infty(\mathbb{R}^3)$. Quasi-free states were introduced by Robinson [17]. They are states which are completely determined by their 1- and 2- point functions. The generating functional of a gauge invariant quasi-free state is of the form

$$\mu(h) = \mu_F(h) \exp\{ -\tfrac{1}{2} Q(h) \} \qquad (2.1)$$

where $Q(\cdot)$ is a positive quadratic form and $\mu_F(h) = \exp\{ -\tfrac{1}{4} \|h\|^2 \}$ is the generating functional of the Fock representation. We assume that $Q(h)$ is closable so that there is a positive self-adjoint operator B whose domain contains $C_c^\infty(\mathbb{R}^3)$ and such that

$$Q(h) = \langle h, Bh \rangle . \tag{2.2}$$

As mentioned earlier, the further assumption that the state determined by (2.1) and (2.2) is Euclidean invariant implies that there is a function $b : \mathbb{R}^+ \to \mathbb{R}^+$ such that

$$B = b(-\Delta) . \tag{2.3}$$

This observation is crucial to our treatment of the problem; it is from here that our approach diverges from those of Fannes [10] and Araki and Lieb [2]. Their methods amount to defining an approximating sequence of normal states by restricting the operator B to $C_c^\infty(\Lambda)$; we restrict the Laplacian, and consider the approximating states determined by $B_\Lambda = b(-\Delta_\Lambda)$. We shall now define this more precisely, following Lewis and Pulè [12].

Let Λ_1 be a bounded region in $\mathbb{R}^3$ with unit volume and which contains the origin. We require the boundary $\partial\Lambda_1$ to satisfy a regularity condition (see sections 3 and 4). For $L > 0$ define

$$\Lambda_L = \{ x \in \mathbb{R}^3 : L^{-1}x \in \Lambda_1 \} , \tag{2.4}$$

Let Δ_L be the Laplacian with domain dense in $L^2(\Lambda_L)$ and with boundary condition

$$\frac{\partial\phi}{\partial n} + \frac{\sigma}{L}\phi = 0 , \tag{2.5}$$

where $\partial/\partial n$ denotes differentiation along the outward normal to the boundary $\partial\Lambda_L$, and σ is a non-negative constant (possibly infinite). Similarly if Λ is a bounded open region with regular boundary then we denote by Δ_Λ the Laplacian on Λ with boundary condition

$$\phi = 0 \quad \text{or} \quad \frac{\partial\phi}{\partial n} + \sigma_\Lambda \phi = 0 , \tag{2.6}$$

σ_Λ being a non-negative constant.

Now define $B_L = b(-\Delta_L)$ and let ω_L be the quasi-free state on $\mathcal{O}(\Lambda_L)$

determined by (2.1) with $Q(h) = \langle h, B_L h \rangle$. ω_L is a normal state if and only if trace $B_L < \infty$ (see Chaiken [5] and Dell'Antonio, Doplicher and Ruelle [9]). But provided b satisfies the conditions of theorem 1 we see that if ω_L is normal then $\omega_{L'}$ is normal for all L' and ω_L (defined using $B_\Lambda = b(-\Delta_\Lambda)$) is normal for any (suitable smooth) region Λ and suitable boundary condition.

In section 4 we prove the following theorem which, from a theorem of Shale [19], amounts to proving that under certain conditions on the function b, ω_L converges to ω in the weak*-topology. (Shale calls this operational convergence.)

THEOREM 2: Let $b : \mathbb{R}^+ \to \mathbb{R}^+$ be the Laplace transform of a positive measure ν for which

(i) $$\int_0^\infty \nu(dt) < \infty ,$$

(ii) $$\int_0^\infty t^{-3/2}\nu(dt) < \infty .$$

Then the generating functional μ_L of ω_L converges to the generating functional μ of ω pointwise in h for $h \in C_c^\infty(\mathbb{R}^3)$.

The condition that b be the Laplace transform of a positive measure can clearly be relaxed to admit those functions b which are Laplace transforms of measures whose positive and negative parts satisfy (i), (ii). To interpret these conditions we note that the particle density $N(\omega)$ is given by

$$N(\omega) = \int_{\mathbb{R}^3} b(|k|^2)\frac{d^3k}{(2\pi)^3} = \int_{\mathbb{R}^3}\left\{\int_0^\infty e^{-t|k|^2}\nu(dt)\right\}\frac{d^3k}{(2\pi)^3} = \int_0^\infty \frac{\nu(dt)}{(2\pi t)^{3/2}} ,$$

so condition (ii) is equivalent to demanding that the state has finite particle density. Furthermore, since ν is positive

$$b(\lambda) \leqslant b(0) = \int_0^\infty \nu(dt)$$

so (i) is equivalent to demanding that b be bounded. This can be interpreted as a 'no-condensation' condition by analogy with various solvable boson gas models where the onset of condensation is accompanied by the relevant density function $b(|k|^2)$ becoming unbounded at 0. (See, for example, Lewis and Pulè [12], Critchley and Lewis [7].)

Having established the convergence of the sequence of states $\{\omega_L\}$ we now return to the problem of the entropy.

THEOREM 3: Let ω be a normal gauge invariant quasi-free state determined by the operator B. Then the entropy $S(\omega)$ of ω is given as follows

(i) if $-\operatorname{trace} B\log B < \infty$ then

$$S(\omega) = \operatorname{trace}\{(1+B)\log(1+B) - B\log B\}$$

(ii) if $-\operatorname{trace} B\log B = \infty$ then

$$S(\omega) = \infty .$$

Note that ω is normal if and only if trace $B<\infty$, and this implies that trace $(1+B)\log(1+B)<\infty$. This theorem can be proved by explicit construction of the corresponding Fock space density matrix ρ_B, and evaluation of ~~-trace~~ $-\operatorname{trace}\rho_B\log\rho_B$. The theorem was proved by Verbeure [21], although his published proof is for Fermi systems. The details in the boson case can be found in [6].

From theorem 3 we see that the entropy of ω_L is

$$S(\omega_L) = \operatorname{trace} \ell\circ b(-\Delta_L)$$

where

$$\ell(t) = (1+t)\log(1+t) - t\log t .$$

This observation enables us to use theorem 1 to prove

THEOREM 4: Let $b: \mathbb{R}^+ \to \mathbb{R}^+$ satisfy the conditions of theorem 1 and be bounded away from zero in any finite subset of $\mathbb{R}^+$. Then $S(\omega_L)$ exists for some L if and only if $\int_{\mathbb{R}^3} \ell\circ b(|k|^2)\,d^3k$ exists. Furthermore if one of these holds then

(i) $S(\omega_L)$ exists for all L.

(ii) $\lim\limits_{L\to\infty} |\Lambda_L|^{-1} S(\omega_L) = \int_{\mathbb{R}^3} \ell\circ b(|k|^2)\dfrac{d^3k}{(2\pi)^3}$.

Proof: The conditions imposed on b ensure that $f = \ell\circ b$ satisfies the conditions of theorem 1. The proof then follows immediately.

We also note that it follows from theorem 1 that if the integral exists then <u>for all</u> scaling sequences of the form (2.4), (2.5), the entropy of every member of each sequence exists, and each sequence of entropy densities converges to the same limit.

Finally in this section we note that any function satisfying the conditions of theorem 2 also satisfies the conditions of theorem 4. This no longer remains true, however, if the positive measure in theorem 2 is replaced by a difference of two positive measures.

§3. A TRACE FORMULA FOR FUNCTIONS OF THE LAPLACIAN

The local Laplacian Δ_Λ, defined in section 2, is an essentially self-adjoint negative operator on $C_c^\infty(\Lambda)$. Its self-adjoint closure, also denoted Δ_Λ, has a spectral decomposition:

$$-\Delta_\Lambda = \int_0^\infty \lambda\, E_\Lambda(d\lambda) . \tag{3.1}$$

Let $F_\Lambda(\lambda) = \operatorname{trace} E_\Lambda(\lambda)$. $F_\Lambda(\lambda)$ is an integer valued function and is equal to the number of eigenvalues of $-\Delta_\Lambda$ less than or equal to λ. It is called the eigenvalue distribution function of $-\Delta_\Lambda$. For the boundary condition (2.5) it can be shown that, provided the boundary is regular enough,

$$\lim_{\lambda\to\infty}\left\{|\Lambda|^{-1}\lambda^{-3/2}F_\Lambda(\lambda)\right\} = \frac{1}{6\pi^2} . \tag{3.2}$$

For a discussion of the regularity properties required to prove this see Mizohata and Arima [14] or McKean and Singer [13]. In section 4 we state a regularity property which we use to prove theorem 2 and for which (3.2) holds.

It follows from (3.2) that there are positive constants $a_\Lambda, b_\Lambda, c_\Lambda, d_\Lambda$ such that

$$a_\Lambda \lambda^{3/2} + b_\Lambda \geq |\Lambda|^{-1} F_\Lambda(\lambda) \geq c_\Lambda \lambda^{3/2} - d_\Lambda \quad . \tag{3.3}$$

(3.2) and (3.3) hold for each member of the sequence of local Laplacians $\{-\Delta_L\}$. But from the scaling (2.4), (2.5) it follows that the eigenvalues scale i.e. ε is an eigenvalue of $-\Delta_1$ if and only if $L^{-2}\varepsilon$ is an eigenvalue of $-\Delta_L$. Therefore if F_L is the eigenvalue distribution function of $-\Delta_L$ then

$$F_L(\lambda) = F_1(L^2\lambda) \tag{3.4}$$

and so (3.3) holds 'uniformly in L' in the following sense :

$$a_1 \lambda^{3/2} + L^{-3} b_1 \geq |\Lambda_L|^{-1} F_L(\lambda) \geq c_1 \lambda^{3/2} - L^{-3} d_1 \quad . \tag{3.5}$$

Furthermore (3.4) and (3.2) imply that pointwise in λ

$$\lim_{L\to\infty} \{ |\Lambda_L|^{-1} F_L(\lambda) \} = (6\pi^2)^{-1} \lambda^{3/2} \quad , \tag{3.6}$$

Motivated by these considerations we make the following definitions:

(1): a positive self-adjoint operator A_Λ whose domain is dense in $L^2(\Lambda)$ $(\Lambda \subset \mathbb{R}^N)$ is said to be a D^N-operator if there are positive constants $a_\Lambda, b_\Lambda, c_\Lambda, d_\Lambda$ such that its eigenvalue distribution function F_Λ satisfies

$$a_\Lambda \lambda^{N/2} + b_\Lambda \geq F_\Lambda(\lambda) \geq c_\Lambda \lambda^{N/2} - d_\Lambda \quad , \tag{3.7}$$

(2): a sequence $\{A_n\}$ of positive self-adjoint operators is said to be a D^N-sequence if

(i) $\mathcal{D}(A_n)$ is dense in $L^2(\Lambda_n)$, $\Lambda_n \subset \mathbb{R}^N$ is bounded.

(ii) there are positive constants a, b, c, d, such that for each n the eigenvalue distribution function F_n of A_n satisfies

$$a\lambda^{N/2} + b \geq |\Lambda_n|^{-1} F_n(\lambda) \geq c\lambda^{N/2} - d \quad . \tag{3.8}$$

(iii) $$\lim_{n\to\infty} |\Lambda_n|^{-1} F_n(\lambda) = \lambda^{N/2} N^{-1} (2\pi)^{-N} S_N \quad , \tag{3.9}$$

where S_N is the surface of the unit sphere in N-dimensions.

From the discussion preceding these definitions it is clear $-\Delta_\Lambda$ is a D^3-operator (for suitable boundary conditions) since an inequality of the form (3.7) can be deduced from an asymptotic property: $F_\Lambda(\lambda) \sim \lambda^{N/2}$ (large λ). Such properties have been extensively studied (see for example Titchmarsh [20] ch. XVII).

Similarly the sequence of local Laplacians $\{-\Delta_L\}$ is a D^N-sequence although the full force of the scaling as reflected in (3.4), (3.5) is not required in (3.8). This suggests that, at least for the proofs of theorems 1 and 4, it may be possible to relax the scaling condition somewhat.

We now state and prove a theorem of which theorem 1 is a particular case.

THEOREM 5: Let A_Λ be a D^N-operator and $\{A_n\}$ a D^N-sequence. Let $f: \mathbb{R}^+ \to \mathbb{R}$ be a bounded differentiable function such that $f' \in L^1_{loc}(\mathbb{R}^+)$ and which is eventually decreasing. Then the following conditions are equivalent:

(i) trace $f(A_\Lambda)$ exists .

(ii) $\int f(|k|^2)\, d^N k$ exists .

(iii) trace $f(A_n)$ exists for each n .

Furthermore if one of the above holds then

$$\lim_{n\to\infty} |\Lambda_n|^{-1} \operatorname{trace} f(A_n) = \int_{\mathbb{R}^N} f(|k|^2)\, d^N k \quad .$$

<u>Proof</u>: Firstly we observe that if f is decreasing and (i), (ii) or (iii) holds then necessarily f is positive and decreasing to zero. Secondly we note that, for the equivalence, it is sufficient to prove that (i) $\Rightarrow$ (ii) and (ii) $\Rightarrow$ (iii), for (iii) $\Rightarrow$ (ii) is the same argument as (i) $\Rightarrow$ (ii), and (ii) $\Rightarrow$ (i) is the same argument as (ii) $\Rightarrow$ (iii). So the proof is split into 3 parts.

(a) : (i) $\Rightarrow$ (ii). The spectral decomposition of A_Λ gives $f(A_\Lambda) = \int_0^\infty f(\lambda) E_\Lambda(d\lambda)$ so that

$$\operatorname{trace} f(A_\Lambda) = \int_0^\infty f(\lambda)\, dF_\Lambda(\lambda). \qquad (3.10)$$

Integrating by parts gives

$$\operatorname{trace} f(A_\Lambda) = -\lim_{R\to\infty} \int_0^\infty f'(\lambda) F_\Lambda(\lambda)\, d\lambda + \lim_{R\to\infty} f(R) F_\Lambda(R) - f(0) F_\Lambda(0). \quad (3.11)$$

But $\lim_{R\to\infty} f(R) F_\Lambda(R) = 0$. To see this let $\{\lambda_n\}$ be the eigenvalues of A_Λ, ordered so that $0 \le \lambda_n \le \lambda_{n+1}$ and counted according to multiplicity. Let $u_n = f(\lambda_n)$, then

$$\Sigma u_n = \operatorname{trace} f(A_\Lambda) < \infty .$$

The hypotheses on f ensure that for all n large enough $0 \le u_{n+1} \le u_n$, so that from a theorem of Olivier [15]

$$\lim n u_n = 0 .$$

But if $F_\Lambda(R) = n$, then $R \ge \lambda_n$ and so (for sufficiently large R) $0 \le f(R) \le f(\lambda_n) = u_n$. Consequently $F_\Lambda(R) f(R) \le n u_n$ and so $\lim_{R\to\infty} F_\Lambda(R) f(R) = 0$. Since $f(0) F_\Lambda(0)$ is finite we deduce that $\int_0^\infty f'(\lambda) F_\Lambda(\lambda)\, d\lambda$ exists and

$$\operatorname{trace} f(A_\Lambda) = -\int_0^\infty f'(\lambda) F_\Lambda(\lambda)\, d\lambda - f(0) F_\Lambda(0). \qquad (3.12)$$

From (3.7)

$$c_\Lambda |f'(\lambda) \lambda^{N/2}| \le |f'(\lambda)| F_\Lambda(\lambda) + d_\Lambda |f'(\lambda)| . \qquad (3.13)$$

Let λ_0 be such that f is decreasing for $\lambda > \lambda_0$ and $F_\Lambda(\lambda_0) \ge 1$. By assumption $|f'|$ and, consequently, $|f'| F_\Lambda$ are integrable over $[0, \lambda_0]$. Furthermore

$$0 \le \int_{\lambda_0}^\infty |f'(\lambda)|\, d\lambda \le \int_{\lambda_0}^\infty |f'(\lambda)| F_\Lambda(\lambda)\, d\lambda = -\int_{\lambda_0}^\infty f'(\lambda) F_\Lambda(\lambda)\, d\lambda .$$

This is finite from (3.12), and so the R.H.S. of (3.13) is integrable; hence the L.H.S. is, and so $f'(\lambda) \lambda^{N/2}$ is. We integrate it by parts and use the fact that $\lim_{R\to\infty} R^{N/2} f(R) = 0$ which follows from another application of (3.7):

$$0 \le |f(R)| R^{N/2} c_\Lambda \le |f(R)| F_\Lambda(R) + d_\Lambda |f(R)| .$$

This gives

$$\begin{aligned}\int_0^\infty \lambda^{N/2} f'(\lambda)\, d\lambda &= -\frac{N}{2} \int_0^\infty f(\lambda) \lambda^{N/2-1}\, d\lambda \\ &= -N \int_0^\infty f(r^2) r^{N-1}\, dr \\ &= \frac{-N}{S_N} \int_{\mathbb{R}^N} f(|k|^2)\, d^N k . \end{aligned} \qquad (3.14)$$

This completes the proof of part (a).

(b) : (ii) $\Rightarrow$ (iii). As in (3.14) (ii) is equivalent to the existence of $\int_0^\infty f(\lambda) \lambda^{N/2-1} d\lambda$. But

$$\begin{aligned}\int_0^\infty f(\lambda) \lambda^{N/2-1}\, d\lambda &= -\lim_{R\to\infty} \frac{2}{N} \int_0^R f'(\lambda) \lambda^{N/2}\, d\lambda + \lim_{R\to\infty} \frac{2}{N} R^{N/2} f(R) \\ &= -\frac{2}{N} \int_0^\infty f'(\lambda) \lambda^{N/2}\, d\lambda \end{aligned} \qquad (3.15)$$

where we have used the fact that

$$\lim_{R\to\infty} R^{N/2} f(R) = 0 \qquad (3.16)$$

which follows from the observation that the integrability of $\lambda^{N/2-1} f(\lambda)$ implies that for large enough

$$\epsilon > \int_{R/2}^R \lambda^{N/2-1} f(\lambda)\, d\lambda > f(R) \left(\frac{R}{2}\right)^{N/2} > 0 .$$

Reversing the argument of part (a) by making extensive use of (3.16) and the left hand half of (3.8) we see that the integrability of $f'(\lambda) \lambda^{N/2}$ (3.15) implies that for each n, $f'(\lambda) F_n(\lambda)$ is integrable and

$$\int_0^\infty f'(\lambda) F_n(\lambda)\, d\lambda = -\int_0^\infty f(\lambda)\, dF_n(\lambda) + f(0) F_n(0) . \tag{3.17}$$

But trace $f(A_n) = \int_0^\infty f(\lambda)\, dF_n(\lambda)$ so this completes the proof of part (b).

(c) : The limit. Lebesgue's dominated convergence theorem and the inequality (3.8) justify the interchange of limit and integration to give

$$\lim_{n\to\infty} |\Lambda_n|^{-1} \operatorname{trace} f(A_n) = \lim_{n\to\infty} -\int_0^\infty f'(\lambda) |\Lambda_n|^{-1} F_n(\lambda)\, d\lambda \qquad \text{from (3.17)}$$

$$= -\int_0^\infty f'(\lambda) \lambda^{N/2}\, d\lambda\, S_N / N(2\pi)^N \qquad \text{from (3.9)}$$

$$= \int_{\mathbb{R}^N} f(|k|^2)\, d^N k/(2\pi)^N . \qquad \text{as in (3.14)}$$

Corollary: Let A_Λ and A_Ω be D^N-operators; then trace $f(A_\Lambda)$ exists if and only if trace $f(A_\Omega)$ exists.

(f, here, is assumed to satisfy the conditions of the theorem.)

§4. PROOF OF THEOREM 2

The proof we give here is a natural generalisation of a proof given by Lewis and Pulè [12] which was developed from an idea by Kac.

Let $h \in C_c^\infty(\mathbb{R}^3)$ then

$$|\mu(h) - \mu_L(h)| = \mu(h)\, |1 - \exp\{\tfrac{1}{2}\langle h, b(-\Delta) h\rangle - \langle h, b(-\Delta_L) h\rangle\}|$$

$$\leq \tfrac{1}{2}\mu(h)\, |\langle h, b(-\Delta) h\rangle - \langle h, b(-\Delta_L) h\rangle| . \tag{4.1}$$

Since b is the Laplace transform of the positive measure ν

$$b(-\Delta) = \int_0^\infty e^{t\Delta}\, \nu(dt)$$

so that the integral kernel $b(-\Delta)[x,y]$ of $b(-\Delta)$ can be expressed in terms of the kernel $G(x,y;t)$ of $e^{t\Delta}$:

$$b(-\Delta)[x,y] = \int_0^\infty G(x,y;t)\, \nu(dt) \tag{4.2}$$

with

$$G(x,y;t) = \exp\{-|x-y|^2/4t\}/(4\pi t)^{3/2} .$$

Similarly

$$b(-\Delta_L)[x,y] = \int_0^\infty G_L(x,y;t)\, \nu(dt) \tag{4.3}$$

where $G_L(x,y;t)$ is the integral kernel of $e^{t\Delta_L}$, i.e. it is the Green's function of the heat equation in Λ_L with boundary condition (2.5). We shall prove the theorem by using estimates of the difference

$$Z_L(x,y;t) = G(x,y;t) - G_L(x,y;t) .$$

Such estimates have been provided by several authors (Mizohata and Arima [14], Arima [3]) for various regularity conditions on the boundary. We choose to follow Angelescu and Nenciu [1] although the proof can be adapted to other cases.

LEMMA. Assume that the boundary $\partial\Lambda_1$ is a C^3 surface of mean curvature less than $1/R$ for some $R > 0$. Then there are constants $K \geq 0, c_1 > 0, c_2 > 0$ such that for all $\sigma \in [0,\infty]$

$$|Z_1(x,y;t)| \leq c_1 \frac{e^{Kt}}{t^{3/2}} \exp\{-c_2 \ell_x^2/t\} \tag{4.4}$$

where

$$\ell_x = \inf_{z\in\partial\Lambda_1} |x - z| .$$

This lemma is a consequence of Propositions A1 and A2 of [1] together with the ordering of Green's functions (in terms of σ) in Remark 2^0 of [1].

As shown by Lewis and Pulè [12], the Green's functions scale:

$$G_L(x,y;t) = L^{-3} G_1(xL^{-1}, yL^{-1}; tL^{-2}) .$$

So from (4.4) we have

$$|Z_L(x,y;t)| \leq c_1 \frac{e^{Kt/2}}{t^{3/2}} \exp\{-c_2 (L\ell_{xL^{-1}})^2/t\} . \tag{4.5}$$

But
$$L\, l_{xL^{-1}} = \inf_{z \in \partial\Lambda_L} |x - z| \,. \tag{4.6}$$

Let $\Omega(h)$ = support h, and let L_0 be chosen so that $\Omega(h)$ is strictly contained in Λ_{L_0}. Then
$$\delta_0 = \inf\{|x-y| : x \in \Omega(h),\, y \in \partial\Lambda_{L_0}\}$$
is strictly positive. Then for $L > L_0$
$$\inf\{|x-z| : x \in \Omega(h),\, z \in \partial\Lambda_L\} \geqslant \frac{L\delta_0}{L_0} \,. \tag{4.7}$$

Now assume that $T > 0$ is fixed. Then gathering together (4.2), (4.3), (4.5), (4.6), (4.7) we have
$$|\langle h, b(-\Delta)h\rangle - \langle h, b(-\Delta_L)h\rangle| = \Big|\iint_{\Omega(h)\times\Omega(h)} dx\,dy \int_0^\infty \overline{h(x)}\, Z_L(x,y;t)\, h(y)\, \nu(dt)\Big|$$
$$\leqslant \int_{\Omega(h)} |h(x)|dx \int_{\Omega(h)} |h(y)|dy \int_0^{TL^2} c_1 \frac{e^{Kt/L^2}}{t^{3/2}} e^{-c_3 L^2/t} \nu(dt)$$
$$+ \int_{TL^2}^\infty \Big|\iint_{\Omega(h)\times\Omega(h)} dx\,dy\, \overline{h(x)}\, h(y)\, Z_L(x,y;t)\Big| \nu(dt) = \mathrm{I} + \mathrm{II} \tag{4.8}$$

where $c_3 = c_2 \delta_0^2 L_0^{-2}$ and
$$\mathrm{I} = c_1 L^{-3} e^{KT} |\hat{h}(0)|^2 \int_0^{TL^2} \frac{e^{-c_3 L^2/t}}{(tL^{-2})^{3/2}} \nu(dt) \,,$$
($\hat{h}(0) = \int_{\mathbb{R}^3} h(x)dx$ is the Fourier transform of h evaluated at zero).

To show that $\mathrm{I} \to 0$ as $L \to \infty$ we note that for any $\beta \in (0, 3/2)$ there is a constant C_4 such that for all $x > 0$
$$c_1 \frac{e^{-c_3 x}}{x^{3/2}} \leqslant \frac{c_4}{x^{3/2-\beta}}$$
so that
$$\mathrm{I} \leqslant c_4 L^{-2\beta} e^{KT} |\hat{h}(0)|^2 \int_0^\infty \frac{\nu(dt)}{t^{3/2-\beta}} \,.$$
But by assumptions (i) and (ii) on ν it follows that the integral is finite and so

$\mathrm{I} \to 0$ as $L \to \infty$. To deal with II we appeal again to Angelescu and Nenciu [1]. Their Remark 2° and Propositions A1 and A3 imply that there is a constant $M(T) > 0$ such that for $t > T$
$$|Z_1(x,y;t)| < M(T) \,.$$
Hence for $t > L^2 T$
$$|Z_L(x,y;t)| = L^{-3} |Z_1(xL^{-1}, yL^{-1}; tL^{-2})| < L^{-3} M(T).$$
Thus
$$\mathrm{II} \leqslant |\hat{h}(0)|^2 M(T) L^{-3} \int_{TL^2}^\infty \nu(dt) \,.$$
This tends to zero by assumption (i) on ν, and completes the proof of Theorem 2.

§5. REMARKS

1°. The set of functions b which satisfy the conditions of the theorems is non-trivial. In particular for the free boson gas above the transition temperature we have
$$b(\lambda) = z(e^{\beta\lambda/2} - z)^{-1}$$
($z \in (0,1)$ is the fugacity, β is the reciprocal of the temperature.) Clearly this satisfies the conditions of theorem 4; it satisfies the conditions of theorem 2 with
$$\nu(dt) = \sum_{n=1}^\infty z^n \delta(t - n\beta/2)\, dt \,.$$

2°. Rocca, Sirugue and Testard [18] showed that a translationally invariant quasi-free KMS state has a two point function determined by an energy spectrum $\epsilon(k)$ and a fugacity z. For a Euclidean invariant state, $\epsilon(k)$ is a function of $|k|^2$; $\epsilon(k) = e(|k|^2)$ so the corresponding b -function is
$$b(\lambda) = \sum z^n e^{-n\beta e(\lambda)} \,.$$
If $z < e^{\beta e(0)}$ and e is differentiable with a completely monotone derivative (in the sense of Feller [11]) then b is the Laplace transform of a positive measure.

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